

# Pekar Ansatz and the Strong Coupling Problem in Polaron Theory.

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## Abstract

A detailed consideration is given to the translation-invariant theory of Tulub polaron constructed without the use of Pekar ansatz. A fundamental result of the theory is that the value of the polaron energy is lower than that obtained on the basis of Pekar ansatz which was considered as an asymptotically exact solution in the strong coupling limit. In the case of bipolarons the theory yields the best values of the coupling energy and critical parameters of their stability. Numerous physical consequences of the existence of translation-invariant polarons and bipolarons are discussed.

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# 1 Introduction. Pekar ansatz.

As is known, polaron theory was among the first to describe the interaction between a particle and a quantum field. Various aspects of the polaron theory are presented in numerous reviews and books [1]-[10]. Being non-relativistic, the theory does not contain any divergencies and for more than sixty years has been a testing area for approbation of various methods of the quantum field theory. Though no exact solution of the polaron problem has been found up to now, it has been believed that the properties of the ground state are known in detail. This primarily refers to the limit cases of weak and strong coupling. A solution in the weak coupling limit was given by Froehlich [11], and that in the strong coupling one was found by Pekar [1],[12]. By now rather an exact solution has been obtained for the energy of the polaron ground state in the weak coupling limit [13],[14] :

$$E_0 = - \left( \alpha + 0.0159196220\alpha^2 + 0.000806070048\alpha^3 + \dots \right) \hbar\omega_0, \quad (1.1)$$

where  $\hbar\omega_0$  is the energy of an optical phonon,  $\alpha$  is the constant of electron-phonon coupling.

A solution of the problem in the opposite strong coupling limit was given by Pekar on the assumption that the wave function  $\Psi$  of the electron + field system has the form:

$$\Psi(r, q_1, \dots, q_i, \dots) = \psi(r)\Phi(q_1, \dots, q_i, \dots), \quad (1.2)$$

where  $\psi(r)$  is the electrons wave function depending only on the electron coordinates,  $\Phi$  – is the wave function of the field depending only on the field coordinates. Pekar himself [1] considered ansatz (1.2) ) to be an approximate solution. In the pioneer works by Bogolyubov and Tyablikov [15],[16] it was shown that in a consistent translation-invariant theory the use of ansatz (1.2) (for decomposed coordinates introduced in [15],[16] ) gives the same results for the polaron ground state energy as the semiclassical Pekar theory does [1],[12]. With the use of (1.2) the value of the ground state energy has been found to a high precision. According to [17],[18] it is equal to::

$$E = \left( -0.108513\alpha^2 - 2.836 \right) \hbar\omega_0. \quad (1.3)$$

The idea that Pekar ansatz (1.2) is an exact solution of the strong coupling polaron problem was completely established after publication of [19] where asymptotics (1.3) was strictly proved by path integral method, i.e. without the use of ansatz (1.2) (see also review [20]).

Before the publication of paper [19] many attempts were made to improve the strong coupling theory [21]-[26]. The reason why Pekar ansatz caused the feeling of disappointment was translation invariance of the initial polaron Hamiltonian. When ansatz for the wave function  $\psi(r)$  (1.2) is used the wave equation has a localized solution. The electron is localized in a potential polarization well induced by it. In other words, the solution obtained does not possess the symmetry of the initial Hamiltonian. Self-trapping of the electron in the localized potential well leads to a spontaneous breaking of the systems symmetry. Attempts to restore the initial symmetry were based on the use of degeneration of the system with broken symmetry. Since in a homogeneous and isotropic medium nothing should depend on the position of the polaron well center  $r_0$ , one can "spread" the initially localized solution over all the positions of the polaron potential well by choosing the wave function in the form of a linear combination in all the positions of the well.

In the most consistent form this program was carried out in [24]. With this end in view for the wave function which is an eigen function of the total momentum, the authors used a superposition of plain waves corresponding to the total momentum multiplied by wave functions obtained from (1.2) to which a translations operator is applied. In other words, they took an appropriate superposition with respect to all the positions of the polaron well  $r_0$ . The main result of paper [24] is that calculation of the polaron ground state energy with such a delocalized function yields the same value as calculations with localized function (1.2) do. The authors of [24] also reproduced the value of the polaron mass which was earlier obtained by Landau and Pekar [27] on the assumption that polaron moves in medium in the localized state (1.2). The results derived in [24] were an important step in resolving the contradiction between the requirement that the translation-invariant wave function be delocalized while the wave function of the self-trapped state be localized.

Notwithstanding the success achieved with this approach it cannot be considered fully adequate since it has quite a few inconsistencies. They follow from the very nature of the semiclassical description used. Indeed, the superposition constructed in [24] on the one hand determines the polaron delocalized state, but on the other hand, without changing this state, one can measure its position and find out a localized polaron well with an electron localized in it. The reason of this paradox is a classical character of the polaron well in the strong coupling limit and, as a consequence, commutation of the total momentum operator with the position of the

polaron well  $r_0$ .<sup>1</sup>

To remedy this defect some approaches were suggested in which the quantity  $r_0(r, q_1, \dots, q_i, \dots)$  which is not actually an additional degree of freedom was considered to be that though with some additional constraints. Discussion of these challenges associated with solution of the problem of introducing collective coordinates is given in review [30]. Since the results obtained by introducing collective coordinates into the polaron theory are polemical it seems appropriate to describe strict results of the translation-invariant theory without recourse to the concept of collective coordinates. The aim of this review is to present an approach used in the strong coupling limit which does not use Pekar ansatz.

A solution possessing these properties in the case of a strong coupling polaron was originally found by Tulub [31],[32]. During nearly half a century the result obtained in [31],[32] was not recognized by specialists working in the field of polaron theory. The reason why the importance of that result was not appreciated was an improper choice of the probe wave function in [32] to estimate the ground state. As a result the ground state energy was found in [32] to be  $E_0 = -0.105\alpha^2\hbar\omega_0$  which is larger than in (1.3). An appropriate choice of the wave function has been made quite recently in paper [33]. This has yielded a lower than in (1.3) value of the polaron ground state energy equal to  $E_0 = -0.125720\alpha^2\hbar\omega_0$ . Hence, actually we have to do with inapplicability of adiabatic approximation in the case of a polaron, though it is fundamental for solid state physics.

In this review we present the main points of the translation-invariant polaron (TI-polaron) theory. In §2 Heisenberg canonical transformation is used to introduce a coordinate-free Pekar Froehlich Hamiltonian which forms the basis for translation-invariant description. With the use of Lee-Low-Pines wave function the weak coupling limit is reproduced.

In §3 we present the general translation-invariant Tulub theory valid for any values of the electron-phonon coupling constant. In view of primary importance of Tulub approach the material is presented in greater detail than in the original paper so that a reader may reproduce and check the results obtained if desired. A general expression is obtained for the TI-polaron

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<sup>1</sup>At the rise of quantum mechanics, the founders of the science were fully aware of the difficulties arising here. Thus, for example, in [28] Bethe notices that for a proper quantum-mechanical description of an interaction between a field and particles, quantizing of the field is required, i.e. quantum theory of the field: "The fact is that, when quantizing mechanical parameters (coordinates and momenta) one should also quantize the associated fields. Otherwise, as Bohr and Rosenfeld showed [29], an imaginary experiment can be suggested which consists in simultaneous measurement of the coordinate and the momentum of a particle from examination of the field induced by it. This contravenes Heisenberg's Uncertainty Principle."

energy for an arbitrary coupling strength.

In §4 a limit case of weak coupling is considered. It is shown that the general expression for the polaron energy derived in the previous section reproduces the weak coupling limit to a high precision.

In §5 a limit case of strong coupling is dealt with. It is shown that in this limit case the polaron ground state energy has a lower value as compared to that obtained on the basis of Pekar ansatz.

In §6 the translation-invariant polaron theory is generalized to the case of a bipolaron. The bipolaron ground state energy obtained here is much lower than that yielded by the best variational calculations with the use of Pekar ansatz. The calculation results are used to explain the high-temperature superconductivity by using TI-bipolarons.

In §7 the energy of TI-polaron and bipolaron is derived in an alternative way. The approach presented there enables one to get an explicit form of wave functions for a polaron and bipolaron. The results obtained suggest that for all the values of the electron-phonon coupling constant the wave functions derived describe delocalized states. Hence it is shown that in the strong coupling limit Pekar ansatz is not fulfilled and no transition to the self-trapped (i.e. localized) state with broken symmetry takes place.

The results obtained radically change the visions of polarons and bipolarons and in the general case cast some doubt on the concept of self-localized states in condensed systems. Recently an open discussion on the completeness of Tulub theory has taken place. The main points and results of the discussion are presented in §8.

In §9 we discuss some problems and consequences emerging from the existence of TI-polarons and bipolarons. Of special practical interest are results concerned with their superconducting properties.

§10 is devoted to discussion of some fundamental problems of the strong coupling theory which are still to be solved.

In Appendices 1-3 we give proofs of some important statements basic to the approach under consideration.

## 2 Coordinate-free Hamiltonian. Weak coupling.

Let us proceed from Pekar-Froehlich Hamiltonian:

$$H = -\frac{\hbar^2}{2m}\Delta_r + \sum_k V_k (a_k e^{ikr} + a_k^\dagger e^{-ikr}) + \sum_k \hbar\omega_k^0 a_k^\dagger a_k, \quad (2.1)$$

where  $a_k^\dagger$ ,  $a_k$  are operators of the birth and annihilation of the field quanta with energy  $\hbar\omega_k^0 = \hbar\omega_0$ ,  $m$  is the electron effective mass,  $V_k$  is a function of the wave vector  $k$ .

Interest in the study of this Hamiltonian is also provoked by the fact that, as distinct from many model Hamiltonians considered in the condensed matter theory, Pekar-Froehlich Hamiltonian (2.1) in the limit of long waves asymptotically exactly describes the behavior of a non-relativistic electron in a continuous polar medium.

Electron coordinates can be excluded from (2.1) via Heisenberg transformation [34]:

$$S_1 = \exp \left\{ \frac{i}{\hbar} \left( \vec{P} - \sum_k \hbar \vec{k} a_k^\dagger a_k \right) \cdot \vec{r} \right\}, \quad (2.2)$$

where  $\vec{P}$  is the total momentum of the system. Application of  $S_1$  to the field operators yields:

$$S_1^{-1} a_k S_1 = a_k e^{-ikr}, \quad S_1^{-1} a_k^\dagger S_1 = a_k^\dagger e^{ikr}.$$

Accordingly the transformed Hamiltonian  $\tilde{H} = S_1^{-1} H S_1$  takes on the form:

$$\tilde{H} = \frac{1}{2m} \left( \vec{P} - \sum_k \hbar \vec{k} a_k^\dagger a_k \right)^2 + \sum_k V_k (a_k + a_k^\dagger) + \sum_k \hbar\omega_k^0 a_k^\dagger a_k. \quad (2.3)$$

Since Hamiltonian (2.3) does not contain electron coordinates, it is obvious that solution of the polaron problem obtained on the basis of (2.3) is translation-invariant. Lee, Low and Pines [35] studied the ground state (2.3) with the probe wave function  $|\Psi\rangle_{LLP}$ :

$$|\Psi\rangle_{LLP} = S_2 |0\rangle, \quad (2.4)$$

where:

$$S_2 = \exp \left\{ \sum_k f_k (a_k^\dagger - a_k) \right\}, \quad (2.5)$$

$f_k$  are variational parameters having the meaning of the value of displacement of the field oscillators from their equilibrium positions,  $|0\rangle$  is the vacuum wave function. The quantity  $f_k$  in  $S_2$  (2.5) is determined by minimization of energy  $E = \langle 0 | S_2^{-1} \tilde{H} S_2 | 0 \rangle$ , which for  $P = 0$  yields:

$$E = 2 \sum_k f_k V_k + \frac{\hbar^2}{2m} \left[ \sum_k \vec{k} f_k^2 \right]^2 + \sum_k \frac{\hbar^2 k^2}{2m} f_k^2 + \sum_k \hbar\omega_k^0 f_k^2, \quad (2.6)$$

$$f_k = -\frac{V_k}{\hbar\omega_k^0 + \hbar^2 k^2 / 2m}. \quad (2.7)$$

In the case of an ionic crystal:

$$V_k = \frac{e}{k} \sqrt{\frac{2\pi\hbar\omega_0}{\varepsilon V}} = \frac{\hbar\omega_0}{ku^{1/2}} \left( \frac{4\pi\alpha}{V} \right)^{1/2}, \quad u = \left( \frac{2m\omega_0}{\hbar} \right)^{1/2}, \quad \alpha = \frac{1}{2} \frac{e^2 u}{\hbar\omega_0 \varepsilon}, \quad \varepsilon^{-1} = \varepsilon_\infty^{-1} - \varepsilon_0^{-1}, \quad (2.8)$$

where  $e$  is an electron charge,  $\varepsilon_\infty$  and  $\varepsilon_0$  are high-frequency and static dielectric permittivities,  $\alpha$  is a constant of electron-phonon coupling. With substitution of (2.8) into (2.6), (2.7) the ground state energy becomes  $E = -\alpha\hbar\omega_0$ , which is the energy of a weak coupling polaron in the first order with respect to  $\alpha$ .

A solution of the problem of transition to the strong coupling case in coordinate-free Hamiltonian (2.3) was found on the basis of the general translation-invariant theory constructed in Tulub's work [32]. The main points of this theory are given in the next section.

### 3 Coordinate-free Hamiltonian. General case.

To construct the general translation-invariant theory in works of [31], [32] was used a canonical transformation of Hamiltonian (2.3) with the use of operator  $S_2$  (2.5) which leads to a shift of the field operators:

$$S_2^{-1} a_k S_2 = a_k + f_k, \quad S_2^{-1} a_k^+ S_2 = a_k^+ + f_k. \quad (3.1)$$

The resultant Hamiltonian  $\tilde{H} = S_2^{-1} \tilde{H} S_2$  has the form:

$$\tilde{H} = H_0 + H_1, \quad (3.2)$$

where:

$$H_0 = \frac{\vec{P}^2}{2m} + 2 \sum_k V_k f_k + \sum_k \left( \hbar\omega_k^0 - \frac{\hbar\vec{k}\vec{P}}{m} \right) f_k^2 + \frac{1}{2m} \left( \sum_k \vec{k} f_k^2 \right)^2 + \mathcal{H}_0, \quad (3.3)$$

$$\mathcal{H}_0 = \sum_k \hbar\omega_k a_k^+ a_k + \frac{1}{2m} \sum_{k,k'} \vec{k}\vec{k}' f_k f_{k'} (a_k a_{k'} + a_k^+ a_{k'}^+ + a_k^+ a_{k'} + a_{k'}^+ a_k), \quad (3.4)$$

$$\hbar\omega_k = \hbar\omega_k^0 - \frac{\hbar\vec{k}\vec{P}}{m} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar\vec{k}}{m} \sum_{k'} \hbar\vec{k}' f_{k'}^2. \quad (3.5)$$

Hamiltonian  $H_1$  contains terms linear, triple and quadruple in the birth and annihilation operators. With an appropriate choice of the wave function diagonalizing quadratic form (3.4)

mathematical expectation  $H_1$  becomes zero (Appendix 1). In what follows we believe that  $\hbar = 1$ ,  $\omega_0 = 1$ ,  $m = 1$ . To transform  $\mathcal{H}_0$  to a diagonal form we put:

$$q_k = \frac{1}{\sqrt{2\omega_k}}(a_k + a_k^+), \quad p_k = -i\sqrt{\frac{\omega_k}{2}}(a_k - a_k^+), \quad \vec{z}_k = \vec{k}f_k\sqrt{2\omega_k}. \quad (3.6)$$

With the use of (3.6) expression (3.4) is written as:

$$\mathcal{H}_0 = \frac{1}{2} \sum_k (p_k^+ p_k + \omega_k^2 q_k^+ q_k) + \frac{1}{2} \left( \sum_k \vec{z}_k q_k \right)^2 - \frac{1}{2} \sum_k \omega_k. \quad (3.7)$$

This yields (3.7) the following motion equation for operator  $q_k$ :

$$\ddot{q}_k + \omega_k^2 q_k = -\vec{z}_k \sum_{k'} \vec{z}_{k'} q_{k'}. \quad (3.8)$$

Let us search for a solution of system (3.8) in the form:

$$q_k(t) = \sum_{k'} \Omega_{kk'} \xi_{k'}(t), \quad \xi_k(t) = \xi_k^0 e^{i\nu_k t}. \quad (3.9)$$

As a result we express matrix  $\Omega_{kk'}$  as:

$$(\nu_{k'}^2 - \omega_k^2) \Omega_{kk'} = \vec{z}_k \sum_{k''} \vec{z}_{k''} \Omega_{k''k'}. \quad (3.10)$$

Let us consider determinant of this system which is derived by replacing the eigenvalues  $\nu_k^2$  in (3.10) with the quantity  $s$  which can differ from  $\nu_k^2$ . The determinant of this system will be

$$\det |(s - \omega_k^2) \delta_{kk'} - \vec{z}_k \vec{z}_{k'}| = \prod_k (s - \nu_k^2). \quad (3.11)$$

On the other hand, according to [36]<sup>2</sup>:

$$\det |(s - \omega_k^2) \delta_{kk'} - \vec{z}_k \vec{z}_{k'}| = \prod_k (s - \omega_k^2) \left( 1 - \frac{1}{3} \sum_{k'} \frac{\vec{z}_{k'}^2}{s - \omega_{k'}^2} \right)^3. \quad (3.12)$$

It is convenient to introduce the quantity  $\Delta(s)$ :

$$\Delta(s) = \prod_k (s - \nu_k^2) / \prod_k (s - \omega_k^2). \quad (3.13)$$

With the use of (3.11) and (3.12)  $\Delta(s)$  is expressed as:

$$\Delta(s) = \left( 1 - \frac{1}{3} \sum_k \frac{\vec{z}_k^2}{s - \omega_k^2} \right)^3. \quad (3.14)$$

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<sup>2</sup>In Wentzel's work  $z_k$  is not a vector function, but a scalar one, therefore a "cube" in (3.12) is lacking. Generalization to the vector case is given in [31].



From (3.11), (3.12) follows that the frequencies  $\nu_k$  renormalized by interaction are determined by a solution to the equation:

$$\Delta(\nu_k^2) = 0. \quad (3.15)$$

The change in the systems energy  $\Delta E$  caused by the electron-field interaction is equal to:

$$\Delta E = \frac{1}{2} \sum_k (\nu_k - \omega_k). \quad (3.16)$$

To express the quantity  $\Delta E$  via  $\Delta(s)$  we use Wentzel approach [36]. Following [36] we write down the identity equation:

$$\begin{aligned} \sum_k \{f(\nu_k^2) - f(\omega_k^2)\} &= \frac{1}{2\pi i} \oint_C ds f(s) \sum_k \left( \frac{1}{s - \nu_k^2} - \frac{1}{s - \omega_k^2} \right) = \\ &= \frac{1}{2\pi i} \oint_C ds f(s) \frac{d}{ds} \ln \Delta(s) = -\frac{1}{2\pi i} \oint_C ds f'(s) \ln \Delta(s), \end{aligned} \quad (3.17)$$

where integration is carried out over the contour presented in Fig.1

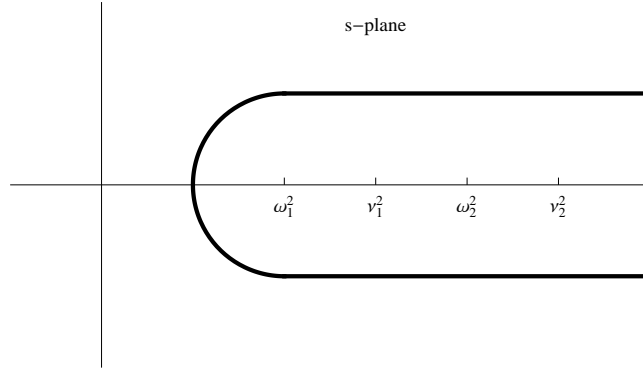


Fig. 1. Contour  $C$ .

Taking  $f(s) = \sqrt{s}$  we get:

$$\Delta E = \frac{1}{2} \sum_k (\nu_k - \omega_k) = -\frac{1}{8\pi i} \oint_C \frac{ds}{\sqrt{s}} \ln \Delta(s). \quad (3.18)$$

Turning in (3.14) from summing up to integration with the use of the relation:

$$\sum_k = \frac{1}{(2\pi)^3} \int d^3k$$

in a continuous case, using for  $\vec{z}_k$  expression (3.14) for  $\Delta(s)$  we obtain:

$$\Delta(s) = D^3(s), \quad D(s) = 1 - \frac{2}{3(2\pi)^3} \int \frac{k^2 f_k^2 \omega_k^2}{s - \omega_k^2} d^3k. \quad (3.19)$$

As a result the total energy of the electron is:

$$E = \Delta E + 2 \sum_k V_k f_k + \sum_k f_k^2 \omega_k^0. \quad (3.20)$$

The results obtained here are general and valid for various polaron models (i.e. any functions  $V_k$  and  $\omega_k^0$ ). Below we consider limit cases of weak and strong coupling which follow from general expression (3.20) on the assumption that  $\vec{P} = 0$ .

Notice that for  $\vec{P} \neq 0$ , according to [31], expression (3.20) takes the form:

$$E = \frac{P^2}{2m} + \Delta E(\vec{P}) + 2 \sum_k V_k f_k + \sum_k \left( \hbar \omega_k^0 - \frac{\hbar \vec{k} \vec{P}}{m} \right) f_k^2 + \frac{1}{2m} \left( \sum_k \vec{k} f_k^2 \right)^2,$$

$$\Delta E(\vec{P}) = -\frac{1}{8\pi i} \oint_C \frac{ds}{\sqrt{s}} \ln \prod_{i=1}^3 D^i(s),$$

$$D^i(s) = 1 - \sum_k \frac{(z_k^i)^2}{s - \omega_k^2},$$

where  $z_k^i$  –  $i$ -th component of the vector  $\vec{z}_k$ . Functions  $f_k$ ,  $\omega_k$  and  $z_k$  are depending on  $|\vec{k}|$  and on  $(\vec{k}\vec{P})$ .

## 4 Weak coupling limit in Tulub theory.

Quantities  $f_k$  in the expression for the total energy  $E$  should be found from the minimum condition:  $\delta E / \delta f_k = 0$  which yields the following integral equation for  $f_k$ :

$$f_k = -V_k / (1 + k^2 / 2\mu_k), \quad \mu_k^{-1} = \frac{\omega_k}{2\pi i} \oint_C \frac{ds}{\sqrt{s}} \frac{1}{(s - \omega_k^2) D(s)}. \quad (4.1)$$

In the case of weak coupling  $\alpha \rightarrow 0$  and equations (4.1) can be solved with the use of perturbation theory. In a first approximation as  $\alpha \rightarrow 0$ ,  $D(s) = 1$  and  $\mu_k^{-1}$  is equal to:

$$\mu_k^{-1} = \frac{\omega_k}{2\pi i} \oint_C \frac{ds}{\sqrt{s}} \frac{1}{(s - \omega_k^2)} = 1. \quad (4.2)$$

Accordingly,  $f_k$  from (4.1) is written as:

$$f_k = -V_k / (1 + k^2 / 2). \quad (4.3)$$

The quantity  $\Delta E$  involved in the total energy takes on the form:

$$\Delta E = -\frac{3}{8\pi i} \oint_C \frac{ds}{\sqrt{s}} \ln D(s), \quad \ln D(s) = -\frac{2}{3(2\pi)^3} \int \frac{k^2 f_k^2 \omega_k}{s - \omega_k^2} d^3 k. \quad (4.4)$$

With the use of (4.3) integrals involved in (4.4) are found to be:  $\Delta E = (\alpha/2)\hbar\omega_0$ . Having calculated the rest of the terms involved in expression (3.20) we get the first term of the expansion of polaron total energy in the coupling constant  $\alpha$ :  $E = -\alpha\hbar\omega_0$ .

In papers [31], [37], [38] a general scheme of calculating the higher terms of expansion in  $\alpha$  was developed. In particular, the eigen energy and effective mass were found to be [38]:

$$\begin{aligned} E &= -(\alpha + 0.01592\alpha^2)\hbar\omega_0, \\ m^* &= \left(1 + \frac{\alpha}{6} + 0.02362\alpha^2\right)m. \end{aligned} \quad (4.5)$$

Hence within the accuracy of the terms  $O(\alpha^3)$  the polaron energy expression calculated within Tulub approach with the use of perturbation theory coincides with exact result (1.1) (see §7).

## 5 Strong coupling.

The case of strong coupling is much more complicated. To reveal the character of the solution in the strong coupling region let us start with considering the analytical properties of the function  $D(s)$  in the form:

$$D(s) = D(1) + \frac{s-1}{3\pi^2} \int_0^\infty \frac{k^4 f_k^2 \omega_k dk}{(\omega_k^2 - 1)(\omega_k^2 - s)}, \quad (5.1)$$

where  $D(1)$  is the value of  $D(s)$  for  $s = 1$ :

$$D(1) = 1 + Q \equiv 1 + \frac{1}{3\pi^2} \int_0^\infty \frac{k^4 f_k^2 \omega_k}{\omega_k^2 - 1} dk. \quad (5.2)$$

From (3.19) also follows that:

$$D(s) = 1 - \frac{1}{3\pi^2} \int_0^\infty \frac{\omega_k k^4 f_k^2}{s - \omega_k^2} dk. \quad (5.3)$$

Function  $D(s)$ , being a function of a complex variable  $s$ , has the following properties: 1)  $D(s)$  has a crosscut along the real axis from  $s = 1$  to  $\infty$  and has no other peculiarities; 2)  $D^*(s) = D(s^*)$ ; 3) as  $s \rightarrow \infty$   $sD(s)$  increases not slower than  $s$ . These properties enable us to present the function  $[(s-1)D(s)]^{-1}$  in the form (Appendix 2):

$$\frac{1}{(s-1)D(s)} = \frac{1}{2\pi i} \oint_{C+\rho} \frac{ds'}{(s'-s)(s'-1)D(s')}, \quad (5.4)$$

where contour  $C + \rho$  is shown in Fig. 2:

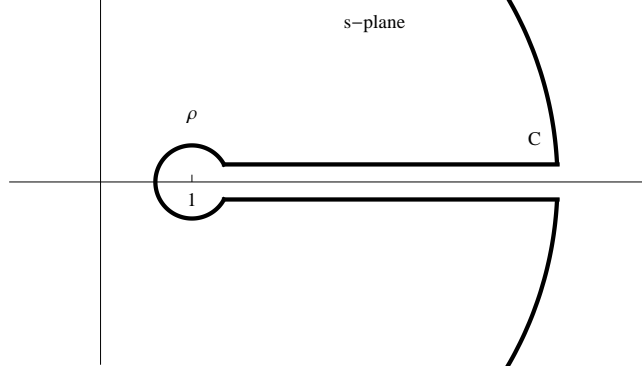


Fig. 2. Contour  $C + \rho$ .

The integrand function in (5.4) has a pole at  $s' = 1$  and a section from  $s' = 1$  to  $s' = \infty$ . Having performed integration in (5.4) along the upper and bottom sides of the crosscut we get the following integral equation for  $D^{-1}(s)$  :

$$\frac{1}{D(s)} = \frac{1}{1+Q} + \frac{s-1}{3\pi^2} \int_0^\infty \frac{k^4 f_k^2 \omega_k dk}{(s - \omega_k^2)(\omega_k^2 - 1)|D(\omega_k^2)|^2}. \quad (5.5)$$

With the use of integration by parts expression (3.18) for  $\Delta E$  can be written as:

$$\Delta E = \frac{1}{2\pi^2} \int_0^\infty dk k^4 f_k^2 \omega_k \frac{1}{2\pi i} \oint_C \frac{\sqrt{s}}{(s - \omega_k^2)^2} \frac{1}{D(s)} ds. \quad (5.6)$$

From (5.5), (5.6) we have:

$$\Delta E = \frac{1}{2\pi^2} \int_0^\infty \frac{k^4 f_k^2 dk}{2(1+Q)} + \frac{1}{12\pi^4} \int_0^\infty \int_0^\infty \frac{k^4 f_k^2 p^4 f_p^2 \omega_p (\omega_k \omega_p + \omega_k(\omega_k + \omega_p) + 1)}{(\omega_k + \omega_p)^2 (\omega_p^2 - 1) |D(\omega_p^2)|^2} dp dk. \quad (5.7)$$

Equation  $\mu_k^{-1}$  (4.1), according to (5.5), can be presented in the form:

$$\mu_k^{-1} = \frac{1}{1+Q} + \frac{1}{3\pi^2} \int_0^\infty \frac{p^4 f_p^2 (\omega_k \omega_p + 1) dp}{(\omega_p^2 - 1)(\omega_k + \omega_p) |D(\omega_p^2)|^2}. \quad (5.8)$$

Equations (4.1), (5.8) for finding  $f_k$  as well as expressions (3.20), (5.7) for calculating polaron energy are very complicated and their exact solution can hardly be obtained. To calculate approximately the energy  $E$  given by (3.20), (5.7) in [32] a direct variational principle was used. For the probe function, the author used Gaussian function of the form:

$$f_k = -V_k \exp(-k^2/2a^2), \quad (5.9)$$

where  $a$  is a variable parameter, besides, as can be seen in the case of strong coupling,  $a \gg 1$ . Substitution of (5.9) into (3.19) yields for real and imaginary parts of  $D(s)$  (see Appendix 3):

$$\begin{aligned} \operatorname{Re} D(\omega_k^2) &= 1 + \lambda v(y), \quad \operatorname{Im} D(\omega_k^2) = k^3 f_k^2 / 6\pi, \\ v(y) &= 1 - ye^{-y^2} \int_0^y e^{t^2} dt - ye^{y^2} \int_y^\infty e^{-t^2} dt, \\ \lambda &= 4\alpha a / 3\sqrt{2\pi}, \quad y = k/a. \end{aligned} \quad (5.10)$$

In the limit of strong coupling ( $\alpha \gg 1$ ) the expression for energy  $E$  given by (3.20) with the use of (5.7) takes on the form:

$$E = \frac{3}{16}a^2 \left[ 1 + q \left( \frac{1}{\lambda} \right) \right] - \frac{\alpha a}{\sqrt{\pi}} \left( 2 - \frac{1}{\sqrt{2}} \right), \quad (5.11)$$

$$q \left( \frac{1}{\lambda} \right) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{e^{-y^2} (1 - \Omega(y)) dy}{(1/\lambda + v(y))^2 + \pi y^2 e^{-2y^2} / 4}, \quad (5.12)$$

$$\Omega(y) = 2y^2 \left\{ (1 + 2y^2) ye^{y^2} \int_y^\infty e^{-t^2} dt - y^2 \right\}.$$

As  $\lambda \rightarrow \infty$ , integral (5.12) has maximum for  $y^4 = 3\lambda/4$ , if the function  $f_k$  is chosen in the form (5.9), however if the actual boundedness of the region of integration with respect to  $y$  is taken into account, this peculiarity does not take place (see §8).

When calculating (5.12) in paper [32] Tulub assumed that in the strong coupling limit  $1/\lambda = 0$ . As a result of numerical integration  $q(0)$  was found to be  $q(0) = 5.75$  whence, varying energy  $E$  (5.11) with respect to  $a$  we get:

$$E = -0.105\alpha^2 \hbar \omega_0. \quad (5.13)$$

Comparison of (5.13) with (1.3) shows that the value of  $E$  obtained for  $\alpha \rightarrow \infty$  lies higher than the exact value in Pekar theory (1.3). For this reason, until quite recently it was believed that Tulub theory as applied to a polaron does not give any new results.

The situation changed radically after publication of [33]. There it was shown that the choice of the wave function for minimizing energy (3.20) in the form (5.9) is not optimal since it does not satisfy virial relations. As is shown in [33], an appropriate function  $f_k$  should contain the multiplier  $\sqrt{2}$  outside the exponent in expression (5.9). Minimization of energy (3.20) with the optimal probe function yields:

$$E = -0.125720\alpha^2 \hbar \omega_0. \quad (5.14)$$

Result (5.14) is fundamental. Above all it means that Pekar ansatz does not give an exact solution. Though result (5.14) refers to a particular case of PekarFroehlich Hamiltonian with  $V_k$  given by (2.8), the conceptual conclusion should be valid for all types of self-localized states. Of special interest is to consider the case of bipolarons since they can play an important role in superconductivity.

## 6 TI-bipolarons.

Great attention given to polaron problem in recent times is associated with attempts to explain the superconductivity phenomenon relying on the mechanism of Bose condensation of bipolaron gas. In this connection the study of conditions under which the bipolaron states are stable is of paramount importance. The theory of large-radius bipolarons which are now considered to be the best candidates for the role of charged bosons forming Bose-Einstein condensate with pairing in real space is considered in detail in reviews [7], [8], [39].

The study of the process of formation of a stable two-electron state in a crystal, or a bipolaron, generally implies finding a pairwise interaction between two polarons as a function of a distance between them [8]. For a large-radius bipolaron, the region of its existence is bordered on the part of the coupling constant  $\alpha$  by rather a large value of  $\alpha_c$  below which the polaron bound state does not exist. In view of the requirement that  $\alpha_c$  be large, which may not be met in high-temperature superconductors, some researchers investigated the contribution of other types of interactions and coupling symmetries [40], [41].

In what follows we will deal with only electron-phonon PekarFroehlich interaction since the approach under consideration can be generalized to other types of interactions as well. It seems all the more actual in view of the fact that in recent times some reasoned arguments have been obtained testifying that electron-phonon interaction in high-temperature superconductors is strong [42]-[44]. There are also arguments in favor of the fact that owing to weak screening of high-frequency optical phonons, the electron-phonon interaction in high-temperature superconductors is more adequately described not in the framework of a contact interaction of Holstein polaron model [45], but in terms of a long-range interaction of Froehlich type [46].

Before the publication of [47]-[49] the lowest values of the energy of bipolaron states determined by electron-phonon interaction were obtained in [50]-[52] for  $\alpha < 8$  and in [52]-[55] for  $\alpha > 8$ . Attempts to find a translation-invariant solution of the bipolaron problem by varia-

tional methods using direct variation of the wave function of the two-electron system [39], [56], [57] yielded higher values of the bipolaron ground state energy as compared to those obtained with the use of a wave function lacking translation invariance [51], [52], [55], [58]. In this section we present the results obtained in [47]-[49] for a bipolaron within the translation-invariant approach.

Let us proceed from Pekar-Froehlich Hamiltonian for a bipolaron [8] :

$$H = -\frac{\hbar^2}{2m}\Delta_{r_1} - \frac{\hbar^2}{2m}\Delta_{r_2} + \sum_k \hbar\omega_k^0 a_k^+ a_k + U(|\vec{r}_1 - \vec{r}_2|) + \sum_k (V_k e^{ikr_1} a_k + V_k e^{ikr_2} a_k + H.C.) , \quad (6.1)$$

$$U(|\vec{r}_1 - \vec{r}_2|) = \frac{e^2}{\varepsilon_\infty |\vec{r}_1 - \vec{r}_2|} ,$$

where  $\vec{r}_1$  and  $\vec{r}_2$  are coordinates of the first and second electrons, respectively, quantity  $U$  describes Coulomb repulsion between the electrons.

In the mass center system Hamiltonian (6.1) takes on the form:

$$H = -\frac{\hbar^2}{2M_e}\Delta_R - \frac{\hbar^2}{2\mu_e}\Delta_r + U(|r|) + \sum_k \hbar\omega_k^0 a_k^+ a_k + \sum_k 2V_k \cos \frac{\vec{k}\vec{r}}{2} \left( a_k e^{i\vec{k}\vec{R}} + H.C. \right) , \quad (6.2)$$

$$\vec{R} = (\vec{r}_1 + \vec{r}_2)/2, \quad \vec{r} = \vec{r}_1 - \vec{r}_2, \quad M_e = 2m, \quad \mu_e = m/2.$$

In what follows we will believe that  $\hbar = 1$ ,  $\omega_k^0 = 1$ ,  $M_e = 1$  (accordingly  $\mu_e = 1/4$ ).

The coordinates of the mass center  $\vec{R}$  can be excluded from Hamiltonian (6.2) via Heisenberg canonical transformation:

$$S_1 = \exp \left\{ -i \sum_k \vec{k} a_k^+ a_k \right\} \vec{R} ,$$

$$\tilde{H} = S_1^{-1} H S_1 = -2\Delta_r + U(|r|) + \sum_k a_k^+ a_k + \sum_k 2V_k \cos \frac{\vec{k}\vec{r}}{2} (a_k + a_k^+) + \frac{1}{2} \left( \sum_k \vec{k} a_k^+ a_k \right)^2 . \quad (6.3)$$

From formula (6.3) follows that the exact solution of the bipolaron problem is determined by the wave function  $\psi(r)$  containing only relative coordinates  $r$  and, therefore, possessing translation invariance.

Averaging of  $\tilde{H}$  over  $\psi(r)$  leads to the Hamiltonian  $\bar{H}$ :

$$\bar{H} = \frac{1}{2} \left( \sum_k \vec{k} a_k^+ a_k \right)^2 + \sum_k a_k^+ a_k + \sum_k \bar{V}_k (a_k + a_k^+) + \bar{T} + \bar{U} , \quad (6.4)$$

$$\bar{V}_k = 2V_k \langle \psi | \cos \frac{\vec{k}\vec{r}}{2} | \psi \rangle , \quad \bar{U} = \langle \psi | U(r) | \psi \rangle , \quad \bar{T} = -2 \langle \psi | \Delta_r | \psi \rangle .$$

Hamiltonian (6.4) differs from Hamiltonian (2.3) in that the quantity  $V_k$  in (2.3) is replaced by  $\bar{V}_k$  and constants  $\bar{T}$  and  $\bar{U}$  are added. Therefore, repeating the derivation performed in §3 we express the bipolaron energy  $E_{bp}$  as:

$$E_{bp} = \Delta E + 2 \sum_k \bar{V}_k f_k + \sum_k f_k^2 + \bar{T} + \bar{U}, \quad (6.5)$$

where  $\Delta E$  is given by expression (5.7). From (6.5) we can get expressions for the bipolaron energy varying  $E_{bp}$  with respect to  $f_k$  and  $\psi$ . Since the equations obtained in this way are difficult to solve, for actual determining of the bipolaron energy we use a direct variational approach, assuming [49]:

$$\begin{aligned} f_k &= -N\bar{V}_k \exp(-k^2/2\mu), \\ \psi(r) &= (2/\pi\ell^2)^{3/4} \exp(-r^2/\ell^2), \end{aligned} \quad (6.6)$$

where  $N$ ,  $\mu$ ,  $\ell$  are variational parameters. For  $N = 1$ , expression (6.6) reproduces the results of work [47], and for  $N = 1$  and  $\mu \rightarrow \infty$ , those of work [48].

Having substituted (6.6) into the expression for the total energy and then minimized the expression obtained with respect to parameter  $N$  we write  $E$  as:

$$\begin{aligned} E(x, y; \eta) &= \Phi(x, y; \eta) \alpha^2, \\ \Phi(x, y; \eta) &= \frac{6}{x^2} + \frac{20.25}{x^2 + 16y} - \frac{16\sqrt{x^2 + 16y}}{\sqrt{\pi}(x^2 + 8y)} + \frac{4\sqrt{2/\pi}}{x(1 - \eta)}. \end{aligned} \quad (6.7)$$

Here  $x$ ,  $y$  are variational parameters:  $x = \ell\alpha$ ,  $y = \alpha^2/\mu$ ,  $\eta = \varepsilon_\infty/\varepsilon_0$ . Let us write  $\Phi_{min}$  for the minimum of function  $\Phi$  of parameters  $x$  and  $y$ . Fig.3 shows the dependence of  $\Phi_{min}$  on the parameter  $\eta$ . Fig.4 demonstrates the dependence of  $x_{min}$ ,  $y_{min}$  on the parameter  $\eta$ .

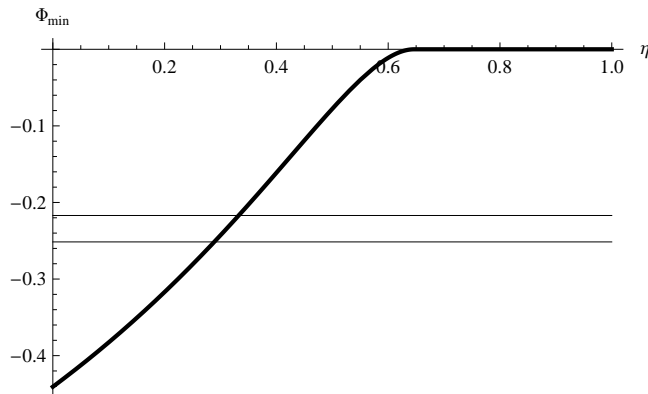


Fig. 3. Graph  $\Phi_{min}(\eta)$ .



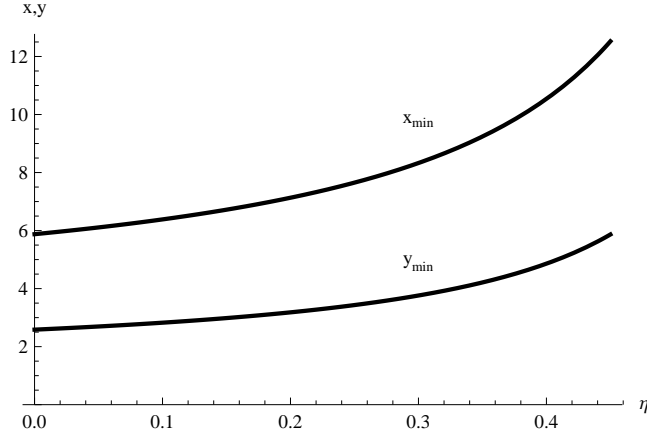


Fig. 4. Graphs  $x_{min}(\eta)$ ,  $y_{min}(\eta)$ .

Fig.3 suggests that  $E_{min}(\eta = 0) = -0.440636\alpha^2$  yields the lowest estimation of the bipolaron ground state energy as compared to all those obtained earlier by variational method. Horizontal lines in Fig.3 correspond to the energies:  $E_1 = -0.217\alpha^2$  and  $E_2 = -0.2515\alpha^2$ , where  $E_1 = 2E_{p_1}$ ,  $E_{p_1}$  is the Pekar polaron ground state energy (1.3);  $E_2 = 2E_{p_2}$  where  $E_{p_2}$  is the ground state energy of a translation-invariant polaron (5.14). Intersection of these lines with the curve  $E_{min}(\eta)$  yields the critical values of the parameters  $\eta = \eta_{c_1} = 0.3325$  and  $\eta = \eta_{c_2} = 0.289$ . For  $\eta > \eta_{c_2}$ , the bipolaron decays into two translation-invariant polarons, for  $\eta > \eta_{c_1}$ , it breaks down into Pekar polarons. The values of minimizing parameters  $x_{min}$  and  $y_{min}$  for these values of  $\eta$  are  $x_{min}(0) = 5.87561$ ,  $y_{min}(0) = 2.58537$ ,  $x_{min}(0.289) = 8.16266$ ,  $y_{min}(0.289) = 3.68098$ ,  $x_{min}(0.3325) = 8.88739$ ,  $y_{min}(0.3325) = 4.03682$ .

The critical value of the electron-phonon coupling constant  $\alpha$ , determined from comparison of the energy expressions in the weak coupling limit (doubled energy of a weak coupling polaron:  $E = -2\alpha\hbar\omega_0$ ) and in the strong coupling limit ( $E = -0.440636\alpha^2\hbar\omega_0$ ), at which the translation-invariant bipolaron is formed is equal to  $\alpha_c \approx 4.54$ , being the lowest estimate obtained by variational method. It should be emphasized that this value is conventional. Hamiltonian (6.4) coincides in structure with one-electron Hamiltonian (2.3), therefore, as in the case of a polaron, the bipolaron energy, by [20], is an analytical function of  $\alpha$ . For this reason at the point  $\alpha = \alpha_c$  the bipolaron energy does not have any peculiarities and the bipolaron state exists over the whole range of  $\alpha$  and  $\eta$  variation:  $0 < \alpha < \infty$ ;  $0 < \eta < 1 - 1/2\sqrt{2}$ , for which  $E < 0$ . To solve the problem of the existence of  $\alpha_c$  value at which the bipolaron state can decay into individual polarons, one should perform calculations for the case of intermediate coupling. In particular, a scenario is possible when the bipolaron energy for some values of  $\eta$  will be lower than the energy

of two individual polarons for all values of  $\alpha$ , i.e. the bipolaron state exists always. Notice, that for the derived state of the translation-invariant bipolaron, the virial theorem holds to a high precision.

The problems of arising high-temperature superconductivity (HTSC) and explaining this phenomenon by formation of bipolaron states were dealt with in a number of papers and reviews [7], [8], [59], [60]. In these works the existence of HTSC is explained by Bose condensation of a bipolaron gas. The temperature of Bose condensation  $T_0 = 3.31\hbar^2 n_0^{2/3} / k_B m_{bp}$ , which is believed to be equal to the critical temperature of a superconducting transition  $T_c$  for  $m_{bp} \approx 10m$ , depending on the bipolarons concentration  $n_0$ , varies in a wide range from  $T_0 = 3K$  at  $n = 10^{18} cm^{-3}$  to  $T_0 \approx 300K$  at  $n \approx 10^{21} cm^{-3}$ . In the latter case the bipolarons concentration is so high that for a bipolaron gas as well as for Cooper pairs, the compound character of a bipolaron when it ceases to behave like an individual particle should show up. In the case of still higher concentrations a bipolaron should decay into two polarons. According to (6.6) the characteristic size of a bipolaron state is equal to  $\ell$  and in dimension units is written as:  $\ell_{corr} = \hbar^2 \tilde{\epsilon} x(\eta) / m e^2$ . Here  $\ell_{corr}$  has the meaning of a correlation length. The dependence  $x(\eta)$  is given by Fig.4. Fig.4 suggests that over the whole range of  $\eta$  variation where the bipolaron state is stable the value of  $x$  changes only slightly: from  $x(\eta = 0) \approx 6$  to  $x(\eta = 0.289) \approx 8$ . Hence, even for  $\eta = \eta_c$ , the critical value of the concentration at which the bipolarons multipiece character is noticeable is of the order of  $n_c \cong 10^{21} cm^{-3}$ . This result testifies that a bipolaron mechanism of HTSC can occur in copper oxides.

## 7 Ground state functional. Tulub ansatz.

To diagonalize quadratic form (3.4) we can use Bogolyubov-Tyablikov transformation [61]. Let us write  $\alpha_k$  for the operators of physical particles in which  $\mathcal{H}_0$  is a diagonal operator.

Let us diagonalize the quadratic form with the use of the transformation:

$$\begin{aligned} a_k &= \sum_{k'} M_{1kk'} \alpha_{k'} + \sum_{k'} M_{2kk'}^* \alpha_{k'}^+, \\ a_k^+ &= \sum_{k'} M_{1kk'}^* \alpha_{k'}^+ + \sum_{k'} M_{2kk'} \alpha_{k'}, \end{aligned} \tag{7.1}$$

so that the equalities:

$$[a_k, a_{k'}^+] = [\alpha_k, \alpha_{k'}^+] = \delta_{kk'}, \quad [H_0, \alpha_k^+] = \omega_k \alpha_k^+. \tag{7.2}$$

be fulfilled.

Relying on the properties of unitary transformation (7.1) we have:

$$\begin{aligned} M_2 M_1^+ &= M_1^* M_2^T, \\ (M_1^+)^{-1} &= M_1 - M_2^* (M_1^*)^{-1} M_2. \end{aligned} \quad (7.3)$$

With the use of (7.3) transformation of the operators reciprocal to (7.1) takes on the form:

$$\begin{aligned} \alpha_k &= \sum_{k'} M_{1kk'}^* a_{k'} - \sum_{k'} M_{2kk'}^* a_{k'}^+, \\ \alpha_k^+ &= \sum_{k'} M_{1kk'} a_{k'}^+ - \sum_{k'} M_{2kk'} a_{k'}. \end{aligned} \quad (7.4)$$

According to [31], [32] matrices  $M_1$  and  $M_2$  are:

$$(M_{1,2})_{kk'} = \frac{1}{2} (\omega_k \omega_{k'})^{-1/2} (\omega_k \pm \omega_{k'}) \left[ \delta(k - k') + (\vec{k} \vec{k}') f_k f_{k'} \frac{2(\omega_k \omega_{k'})^{1/2}}{(\omega_{k'}^2 - \omega_k^2 \pm i\varepsilon) D_{\pm}(\omega_k^2)} \right], \quad (7.5)$$

$$D_{\pm}(\omega_p^2) = 1 + \frac{1}{3\pi^2} \int_0^{\infty} \frac{f_k^2 k^4 \omega_k}{\omega_k^2 - \omega_p^2 \mp i\varepsilon} dk,$$

where the superscript sign in the right-hand side of (7.5) refers to  $M_1$  and the subscript sign to  $M_2$ . As a result of diagonalization quadratic form (3.4) changes to:

$$\mathcal{H}_0 = \Delta E + \sum_k \nu_k \alpha_k^+ \alpha_k. \quad (7.6)$$

Functional of the ground state  $\Lambda_0|0\rangle$  is chosen from the condition:

$$\alpha_k \Lambda_0|0\rangle = 0. \quad (7.7)$$

The explicit form of functional  $\Lambda_0$  is conveniently derived if we use Fock representation for operators  $a_k$  and  $a_k^+$  [62], [63] which associates operator  $a_k^+$  with some  $c$ -number  $\bar{a}_k$  and operator  $a_k$  with operator  $d/d\bar{a}_k$ . Then, with the use of (7.4) condition (7.7) takes on the form:

$$\left( \sum_{k'} M_{1kk'}^* \frac{d}{d\bar{a}_{k'}} - \sum_{k'} M_{2kk'}^* \bar{a}_{k'} \right) \Lambda|0\rangle = 0. \quad (7.8)$$

It is easy to verify by direct substitution in (7.8) that solution of equation (7.8) is written as:

$$\Lambda_0 = C \exp \left\{ \frac{1}{2} \sum_{k,k'} a_k^+ A_{kk'} a_{k'}^+ \right\}, \quad (7.9)$$

where  $C$  is a constant. To this end it is sufficient to return in (7.9) to quantities  $\bar{a}_k$  instead of  $a_k^+$ . Matrix  $A$  satisfies the conditions:

$$A = M_2^* (M_1^*)^{-1}, \quad A = A^T. \quad (7.10)$$

Hence, the ground state energy corresponding to functional  $\Lambda_0$  is equal to:

$$\langle 0 | \Lambda_0^+ \mathcal{H}_0 \Lambda_0 | 0 \rangle = \Delta E. \quad (7.11)$$

In Appendix 1 we show that  $\langle 0 | \Lambda_0^+ H_1 \Lambda_0 | 0 \rangle \equiv 0$ .

From (7.9), (2.2), (2.5) it follows that the wave function of the polaron ground state  $|\psi\rangle_p$  has the form:

$$|\psi\rangle_p = C e^{-\frac{i}{\hbar} \sum_k \hbar \vec{k} a_k^+ a_k \vec{r}} e^{\sum_k f_k (a_k^+ - a_k)} \Lambda_0 |0\rangle. \quad (7.12)$$

Accordingly the bipolaron wave function  $|\psi\rangle_{bp}$ , with regard to (5.3), (5.4) is:

$$|\psi\rangle_{bp} = C \psi(r) e^{-\frac{i}{\hbar} \sum_k \hbar \vec{k} a_k^+ a_k \vec{R}} e^{\sum_k f_k (a_k^+ - a_k)} \Lambda_0 |0\rangle. \quad (7.13)$$

Formula (7.12), (7.13) imply that the wave functions of a polaron and bipolaron are delocalized over the whole space and cannot be presented as an ansatz (1.2).

From formulae (7.12), (7.13) it follows that the reason why the attempt of Lee, Low and Pines [35] to investigate the polaron ground state energy over the whole range of  $\alpha$  variation failed was an improper choice of probe function (2.4) which lacks the multiplier corresponding to the functional  $\Lambda_0$ .

However, it should be stressed that notwithstanding a radical improvement of the wave function achieved by introducing the multiplier  $\Lambda_0$  in Lee, Low, Pines function enables one to take account of both weak and strong coupling, the results obtained by its application are not exact. The fact that Tulub function is an ansatz follows from its properties:

$$\langle 0 | \Lambda_0^+ H_1 \Lambda_0 | 0 \rangle = 0, \quad E = \langle 0 | \Lambda_0^+ H_0 \Lambda_0 | 0 \rangle, \quad H_0 \Lambda_0 | 0 \rangle = E \Lambda_0 | 0 \rangle. \quad (7.14)$$

Being an ansatz, Tulub's solution presents a solution of the polaron problem in a specific class of functions having the structure of  $\Lambda_0 |0\rangle$ . That Tulub ansatz is not an exact solution of the problem follows at least from the fact that the use of expression (3.20) alone for calculation of the energy, for example, in the case of weak coupling yields for  $E$ :  $E = -\alpha - \frac{1}{6} \left( \frac{1}{2} - \frac{4}{3\pi} \right) \alpha^2$  [31]. To get an exact coefficient at  $\alpha^2$  in the expansion of the energy in powers of  $\alpha$  (1.1) we should take into account the contribution of Hamiltonian  $H_1$ , as the perturbation theory suggests [38].

The fact that wave functions (7.12), (7.13) are delocalized has a lot of important consequences which will be discussed in Section 9.

## 8 Discussion of the completeness of Tulub theory.

In [64], [65] a question was raised as to whether Tulub theory [31], [32] is complete. Arguments of [64], [65] are based on the work by Porsch and Röseler [37] which reproduces the results of Tulub theory. However, in the last section of their paper Porsch and Röseler investigate what will happen if the infinite integration limit in Tulub theory changes for a finite limit and then passes on to the infinite one. Surprisingly, it was found that in this case in parallel with cutting of integration to phonon wave vectors in the functional of the polaron total energy one should augment the latter with the addition  $\delta E^{PR}$  which input will not disappear if the upper limit tends to infinity [37], [65]. Relying on this result the authors of [64], [65] concluded that Tulub did not take this addition into account and therefore his theory is incomplete.

To resolve this paradox let us consider the function  $\Delta(s)$  determined by formula (3.14) (accordingly, (3.19) in continuous case). As formulae (3.14), (3.19) imply, zeros in this function contribute into "polaron recoil" energy  $\Delta E$  given by (3.16) and, according to (3.15) are found from the solution of the equation:

$$1 = \frac{2}{3} \sum_k \frac{k^2 f_k^2 \omega_k}{s - \omega_k^2}. \quad (8.1)$$

If the cutoff is absent in the sum on the right-hand side of equation (8.1), then the solution of this equation yields a spectrum of  $s$  values determined by frequencies  $\nu_{k_i}$  lying between neighboring values of  $\omega_{k_i}$  and  $\omega_{k_{i+1}}$  for all the wave vectors  $k_i$ . These frequencies determine the value of the polaron recoil energy:

$$\Delta E = \frac{1}{2} \sum_{k_i} (\nu_{k_i} - \omega_{k_i}). \quad (8.2)$$

Let us see what happens with the contribution of frequencies  $\nu_{k_i}$  into  $\Delta E$  in the region of the wave vectors  $k$  where  $f_k$  vanishes but nowhere becomes exactly zero. From (8.1) it follows that as  $f_k \rightarrow 0$ , solutions of equation (8.1) will tend to  $\omega_{k_i}$ :  $\nu_{k_i} \rightarrow \omega_{k_i}$ . Accordingly, the contribution of the wave vectors region into  $\Delta E$ , where  $f_k \rightarrow 0$ , will also tend to zero.

In particular, if we introduce a certain  $k^0$  such that in the region  $k > k^0$  the values of  $f_k$  are small, we will express  $\Delta E$  in the form:

$$\Delta E = \frac{1}{2} \sum_{k_i \leq k^0} (\nu_{k_i} - \omega_{k_i}), \quad (8.3)$$

which does not contain any additional terms. To draw a parallel with Tulub approach, there we could put the upper limit  $k^0$ , but no additional terms would appear.

For example, if in an attempt to investigate the minimum of Tulub functional (3.20), (5.7) we choose the probe function  $f_k$  not containing a cutoff in the form [49]:

$$\begin{aligned} f_k &= -V_k \exp(-k^2/2a^2(k)), \\ a(k) &= \frac{a}{2} \left[ 1 + \text{th} \left( \frac{k_b - k}{a} \right) \right], \end{aligned} \quad (8.4)$$

where  $a$  is a parameter of Tulub probe function (5.9),  $k_b$  satisfies the condition  $a \ll k_b \ll k_{oc}$ ,  $k_{oc} = a\sqrt[4]{3\lambda/4}$  is the value of the wave vector for which Tulub integral (5.12) has a maximum [32], [66], then with the use of (8.4) in the limit  $a \rightarrow \infty$ , Tulub integral  $q(1/\lambda)$  will be written as:

$$q\left(\frac{1}{\lambda}\right) \approx 5.75 + 6 \left(\frac{a}{k_b}\right)^3 \exp\left(-\frac{k_b^2}{a^2}\right). \quad (8.5)$$

The second term in the right-hand side of (8.5) vanishes as  $k_b/a \rightarrow \infty$  and we get, as we might expect, Tulubs result:  $q(1/\lambda) \approx 5.75$ .

Equation (8.1), however, has a peculiarity. Even in the case of a continuous spectrum, for  $f_k = 0$ , if  $k > k^0$  it has an isolated solution  $\nu_{k^0}$  which differs from the maximum frequency  $\omega_{k^0}$  by a finite value. This isolated solution leads to an additional contribution into  $\Delta E$ :

$$\begin{aligned} \Delta E &= \frac{1}{2} \sum_{k_i < k^0} (\nu_{k_i} - \omega_{k_i}) + \delta E^{PR}, \\ \delta E^{PR} &= \frac{3}{2} (\nu_{k^0} - \omega_{k^0}), \end{aligned} \quad (8.6)$$

where  $\nu_{k^0}$  has the meaning of "plasma frequency" [37]. Hence, here a continuous transition from the case of  $f_k \rightarrow 0$  for  $k > k^0$  to the case of  $f_k = 0$  for  $k > k^0$  is absent. As is shown by direct calculation [67], of the contribution of the term with "plasma frequency"  $\delta E^{PR}$  into (8.6), even for  $k^0 \rightarrow \infty$ , Porsch and Röseler theory does not transform itself into Tulub theory.

In Tulub theory we choose such  $f_k$  which lead to the minimum of the functional of the polaron total energy. In particular, the choice of the probe function in the form (8.4) provides the absence of a contribution from "plasma frequency" into the total energy and in actual calculations one can choose a cutoff  $f_k$  without introducing any additional terms in Tulub functional [66], [67].

To sum up, critical remarks in [64], [65] are inadequate. Their inadequacy was demonstrated in papers [66], [67] and in work [49] reproduced here. At the present time Tulub theory and the results obtained on its basis [33], [47]-[49] give no rise to doubt.

## 9 Consequences of the existence of translation-invariant polarons and bipolarons.

According to the results obtained, the ground state of a TI-polaron is a delocalized state of the electron-phonon system: the probabilities of electrons occurrence at any point of the space are similar. The explicit form of the wave function of the ground state is presented in §7. Both the electron density and the amplitudes of phonon modes (corresponding to renormalized by interaction frequencies  $\nu_{q_i}$ ) are delocalized.

It should be noted that according to (3.15) renormalized phonon frequencies  $\nu_{q_i}$  in the case of a TI-polaron have higher energies than non-renormalized frequencies of optical phonons and, therefore, higher energies than non-renormalized frequencies of a polaron with spontaneously broken symmetry [68]. This holds out a hope to find such phonon modes in experiments on light combination scattering and optical absorption. According to [68], if a polaron (bipolaron) is bound on the Coulomb center, i.e. it forms an  $F$ -center ( $F'$ -center), then all renormalized local phonon frequencies  $\omega_n$  have lower energies than the frequency of optical phonon  $\omega_0$  does. This fact also makes easier experimental validation of the occurrence of delocalized TI-phonon modes with  $\nu_{q_i} > \omega_0$ .

The concept of a polaron potential well (formed by local phonons [68]) in which an electron is localized, i.e. the self-trapped state is lacking in the translation-invariant theory. Accordingly, the induced polarization charge of the TI-polaron is equal to zero. Polarons lacking a localized "phonon environment" suggests that its effective mass is not very much different from that of an electron. The ground state energy of a TI-polaron is lower than that of Pekar polaron and is given by formula (5.14) (for Pekar polaron the energy is determined by (1.3)).

Hence, for zero total momentum of a polaron, there is an energy gap between the TI-polaron state and the Pekar one (i.e. the state with broken translation invariance). The TI-polaron is a structureless particle (the results of investigations of the Pekar polaron structure are summed up in [68]).

According to the translation-invariant polaron theory, the terms "large-radius polaron" (LRP) and "small-radius polaron" (SRP) are relative, since in both cases the electron state is delocalized over the crystal. The difference between the LRP and SRP in the translation-invariant theory lies in the fact that for the LRP the inequality  $k_{char}a < \pi$  is fulfilled, while for

the SRP  $k_{char}a > \pi$  holds, where  $a$  is the lattice constant and  $k_{char}$  is a characteristic value of the phonon wave vectors making the main contribution into the polaron energy. This statement is valid not only for Pekar-Froehlich polaron, but for the whole class of polarons whose coupling constant is independent of the electron wave vector, such as Holstein polaron, for example. For polarons whose coupling constant depends on the electron wave vector, these criteria may not hold (as is the case with Su-Schreiffer-Heeger model, for example [69]).

These properties of TI-polarons determine their physical characteristics which are qualitatively different from those of Pekar polarons. When a crystal has minor local disruptions, the TI-polaron remains delocalized. For example, in an ionic crystal containing vacancies, delocalized polaron states will form  $F$ -centers only at a certain critical value of the static dielectric constant  $\varepsilon_{0c}$ . For  $\varepsilon_0 > \varepsilon_{0c}$ , a crystal will have delocalized TI-polarons and free vacancies. For  $\varepsilon_0 = \varepsilon_{0c}$ , a transition from the delocalized state to that localized on vacancies (collapse of the wave function) will take place. Such behavior of translation-invariant polarons is qualitatively different from that of Pekar polarons which are localized on the vacancies at any value of  $\varepsilon_0$ . This fact accounts for, in particular, why free Pekar polaron does not demonstrate absorption (i.e. structure), since in this case the translation-invariant polaron is realized. Absorption is observed only when a bound Pekar polaron, i.e.  $F$ -center is formed. These statements are also supported by a set of recent papers where Holstein polaron is considered [70]-[72]. The approach presented is generalized by the author to the case of Holstein polaron in [73].

Notice that the physics of only free strong-coupling polarons needs to be changed. The overwhelming majority of results on the physics of strong-coupling polarons has been obtained for bound (on vacancies or lattice disruptions) polaron states of Pekar type and do not require any revision.

Taking account of translation invariance in the case of a polaron leads to a minor change in the assessment of the ground state, however leads to qualitatively different visions of the properties of this state. In paper [32], in the section devoted to scattering of a TI-polaron, Tulub shows that as the constant of electron-phonon coupling increases up to a certain critical value, scattering of an electron on optical phonons turns to zero. Hence, when the coupling constants exceed a critical value a polaron becomes superconducting. Though in ionic crystals the main mechanism of electron scattering is scattering on optical phonons [74], it might appear that the contribution of acoustic phonons should also be taken into account in this case. However, as



it follows from the law of conservation of energy and momentum, a TI-polaron will scatter on acoustic phonons only if its velocity exceeds that of sound [75].

As distinct from polarons, TI-bipolarons have much greater binding energy. This leads to some important physical consequences. In particular, when a crystal has minor local disruptions, a TI-bipolaron will be delocalized. Thus, in an ionic crystal with lattice vacancies, formation of  $F'$ -centers by delocalized bipolarons will take place only at a certain critical value of the static dielectric constant  $\varepsilon_{0c1}$ . For  $\varepsilon_0 > \varepsilon_{0c1}$ , the crystal will contain delocalized TI-bipolarons and free vacancies. In the case of  $\varepsilon_0 = \varepsilon_{0c1}$  TI-bipolarons will pass on from the delocalized state to that localized on vacancies, i.e. to  $F'$ -center. Such behavior of TI-bipolarons is qualitatively different from the behavior of polarons with spontaneously broken symmetry of Pekar type [8], which are localized on the vacancies at any value of  $\varepsilon_0$ .

The fundamental difference between TI-bipolarons and bipolarons with spontaneously broken symmetry is that the former are not separable while the latter are separable. This is due to the fact that in the case of bipolarons with spontaneously broken symmetry interaction between electrons and polarization has the form:  $\Phi(\vec{r}_1, \vec{r}_2) = F(\vec{r}_1) + F(\vec{r}_2)$ . For  $|\vec{r}_1 - \vec{r}_2| \gg R$ , where  $R$  is the bipolaron radius, bipolaron equations separate into two independent polaron equations. This fact enables us to treat a bipolaron state with spontaneously broken symmetry as a bound state of two polarons [8]. In the case of TI-bipolarons:  $\Phi(\vec{r}_1, \vec{r}_2) = \Phi(\vec{r}_1 - \vec{r}_2)$ . In this case, splitting of the bipolaron interaction functional into the functionals of interaction of individual polarons is impossible for any  $|\vec{r}_1 - \vec{r}_2|$  and treatment of TI-bipolarons as composite states becomes invalid. This conclusion corresponds to modern ideas that a quantum-mechanical system cannot be separated into independent subsystems [76].

For zero total momentum of a bipolaron, TI-bipolarons, being delocalized, will be separated from those with broken translation invariance by an energy gap. As with TI-polarons, in the case when the coupling constant exceeds a certain critical value, TI-bipolarons become superconducting. As is known, interpretation of the high-temperature superconductivity relying on the bipolaron mechanism of Bose-condensation runs into a problem associated with a great mass of bipolarons and, consequently low temperature of Bose-condensation. The possibility of smallness of TI-bipolarons mass resolves this problem. It should be stressed that the above-mentioned properties of translation-invariant bipolarons impart them superconducting properties even in the absence of Bose-condensation, while the great binding energy of

bipolarons substantiates the superconductivity scenario even in badly defect crystals.

## 10 Conclusive remarks.

At the present time Tulub theory and quantitative results obtained on its basis give no rise to doubt. The quantum field theory under consideration is nonperturbative and can reproduce not only the limits of weak and strong coupling but also the case of intermediate coupling.

One of the most effective methods for calculating polarons and bipolarons in the case of intermediate coupling is integration over trajectories [77]. Unless properly modified, this approach is not translation-invariant since in this method the main contribution into the energy levels is given by classical solutions (i.e. extrema points of the exponent of classical action, involved in the path integral). However, such solutions, in view of translation invariance, are not isolated stationary points, but belong to a continuous family of classical solutions obtained as a result of action of the translation operator on the initial classical solution. Accordingly, the stationary phase approximation is inapplicable in the translation-invariant system. In the quantum field theory some approaches are developed for restoring translation invariance. They are based on introducing collective coordinates into the functional integral [78]. However, they have not been used in the polaron theory as yet. Therefore it is not surprising that the method of integrals over trajectories employed in the plaron theory yields a result coinciding with the semiclassical theory of the strong coupling polaron [79].

Recently in the polaron theory a powerful computational method, namely Monte-Carlo technique has been developed [80], [81]. This procedure, being only a calculation tool, cannot reproduce the results of Tulub ansatz unless properly modified. As for Monte-Carlo diagram technique, the obstacle to checking Tulub ansatz in the strong coupling limit is presented by the necessity to calculate diagrams of very high order.

To sum up, Pekar ansatz (1.2) provides an original assumption of the form of the solution which was confirmed in the course of numerous examinations. For nearly eighty-year history of the polaron theory development (if dating from Landau short paper [82]) ansatz (1.2) has been recognized to be an asymptotically exact solution of the polaron problem in the strong coupling limit.

Tulub ansatz (§7) provides another assumption of the form of the solution whose structure is determined by the form of the function  $\Lambda_0|0\rangle$ . In terms of this assumption Tulub solution is

also asymptotically exact. Since Tulub solution yields a lower energy value for a polaron, from the variational standpoint, preference should be given to Tulub ansatz.

Hence, polaron theory in no way can be considered to be complete. In the framework of Tulub ansatz great work is to be done to revise many concepts (such as superconductivity) in condensed matter physics. Extension of the application area of Tulub ansatz to other divisions of the quantum field theory can lead to radical revision of many results which nowadays seem doubtless and vice-versa. Thus, for example, non-separability of a bipolaron state in the polaron model of quarks [83] (the role of phonons in [83] is played by a gluon field) provides a natural explanation of their confinement. In paper [73] it is noted, that in TI-theory there is no need to use Higgs mechanism of spontaneous symmetry breaking to get the elementary particles masses.

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## Appendix 1.

Hamiltonian  $H_1$  involved in (3.2) has the form:

$$H_1 = \sum_k (V_k + f_k \hbar \omega_k) (a_k + a_k^\dagger) + \sum_{k,k'} \frac{\vec{k} \vec{k}'}{m} f_{k'} (a_k^\dagger a_k a_{k'} + a_k^\dagger a_{k'}^\dagger a_k) + \frac{1}{2m} \sum_{k,k'} \vec{k} \vec{k}' a_k^\dagger a_{k'}^\dagger a_k a_{k'}, \quad (A1.1)$$

where  $\hbar \omega_k$  is given by expression (3.5). Let us apply the operator  $H_1$  to functional  $\Lambda_0$  (7.9). We will show that  $\langle 0 | \Lambda_0^+ H_1 \Lambda_0 | 0 \rangle = 0$ . Indeed, the action of  $\Lambda_0$  on  $H_1$  terms containing an odd number of operators in  $H_1$  (i.e. the first and second terms in  $H_1$ ) will always contain an odd number of terms and mathematical expectation for these terms will tend to zero.

Let us consider mathematical expectation for the last term in  $H_1$ :

$$\langle 0 | \Lambda_0^+ \sum_{k,k'} \vec{k} \vec{k}' a_k^\dagger a_{k'}^\dagger a_k a_{k'} \Lambda_0 | 0 \rangle. \quad (A1.2)$$

The function  $\langle 0 | \Lambda_0^+ a_k^\dagger a_{k'}^\dagger a_k a_{k'} \Lambda_0 | 0 \rangle$  represents the norm of vector  $a_k a_{k'} \Lambda_0 | 0 \rangle$  and will be positively defined for all  $k$  and  $k'$ . If we replace  $\vec{k} \rightarrow -\vec{k}$  in (A1.2) than the whole expression will change the sign and, therefore, (A1.2) is also equal to zero. Hence  $\langle 0 | \Lambda_0^+ H_1 \Lambda_0 | 0 \rangle = 0$ .

## Appendix 2.

Let us show that (5.4), (5.5) follow from (5.1), (5.2). To this end notice that analytical properties of  $D(s)$  pointed out in [32] straightforwardly follow from (3.19). Indeed, the pole of  $D(s)$  can lie only on the real axis since in view of positive definedness of  $\omega_k k^4 f_k^2$  in (3.19) equation:

$$1 + \frac{1}{3\pi^2} \int_0^\infty \frac{\omega_k k^4 f_k^2 (\omega_k^2 - s_0 + i\varepsilon)}{(\omega_k^2 - s_0)^2 + \varepsilon^2} dk = 0, \quad (A2.1)$$

can be fulfilled only for  $\varepsilon = 0$ . Besides,  $D(s)$  is a monotonously increasing function  $s$  since for  $s < 1$ ,  $D'(s) > 0$ , and as  $s_0 \rightarrow \infty$ ,  $D(s)$  turns to unit. Therefore  $D(s)$  cannot have zeros for  $-\infty < s_0 < 1$ . Hence function  $(s - 1)D(s)$  can be presented in the form:

$$\frac{1}{(s - 1)D(s)} = \frac{1}{2\pi i} \oint_{C+\rho} \frac{ds'}{(s' - s)(s' - 1)D(s')}, \quad (A2.2)$$

where the contour of integration in Cauchy integral (A2.2) is shown in Fig.2. The integrand function in (A2.2) has a pole for  $s' = 1$  and a section from  $s' = 1$  to  $s' \rightarrow \infty$ . Performing integration in (A2.2) with respect to the upper and bottom sides of the crosscut we will get integral equation (5.5).

## Appendix 3.

Let us perform a detailed calculation of the quantity  $\Delta E$  (5.7) with the use of probe function (5.9).

To this end, to calculate the real part of  $D(\omega_p^2)$  involved in (5.7) we use Sokhotskys formula:

$$\frac{1}{\omega_k^2 - \omega_p^2 - i\varepsilon} = \mathcal{P} \frac{1}{\omega_k^2 - \omega_p^2} + i\pi\delta(\omega_k^2 - \omega_p^2),$$

$$\text{Re } D(\omega_p^2) = 1 + \frac{1}{3\pi^2} \int_0^\infty f_k^2 k^4 \mathcal{P} \frac{\omega_k}{\omega_k^2 - \omega_p^2} dk.$$

It is convenient to present  $\text{Re } D$  in the form:

$$\text{Re } D = 1 + I_1 + I_2,$$

$$I_1 = \frac{1}{3\pi^2} \int_0^\infty f_k^2 k^4 \frac{dk}{\omega_k + \omega_p}, \quad I_2 = \mathcal{P} \frac{\omega_p}{3\pi^2} \int_0^\infty \frac{f_k^2 k^4 dk}{(\omega_k - \omega_p)(\omega_k + \omega_p)}.$$

Substituting  $f_k$  in the form of (5.9) into these expressions we present  $I_1$  as:

$$I_1 = \frac{8\alpha}{3\sqrt{2}\pi} \int_0^\infty e^{-k^2/a^2} dk - \frac{8\alpha(p^2+4)}{3\sqrt{2}\pi} \int_0^\infty \frac{e^{-k^2/a^2}}{k^2+p^2+4} dk.$$

Assuming  $k/a = \tilde{k}$  in the strong coupling limit ( $a \rightarrow \infty$ ) we write for  $I_1$ :

$$I_1 = \frac{8\alpha a}{3\sqrt{2}\pi} \left[ \frac{\sqrt{\pi}}{2} - \frac{\pi}{2} \tilde{p} e^{\tilde{p}^2} \left( 1 - \frac{2}{\sqrt{\pi}} \int_0^{\tilde{p}} e^{-t^2} dt \right) \right].$$

Accordingly,  $I_2$  takes on the form:

$$I_2 = \mathcal{P} \frac{4\alpha\omega_p}{3\pi\sqrt{2}} \int_0^\infty \frac{e^{-k^2/a^2} k^2 dk}{(\omega_k - \omega_p)(\omega_k + \omega_p)}.$$

This integral can be expressed as:

$$I_2 = I_{20} + I_{21},$$

where:

$$I_{20} = \frac{16\alpha\omega_p}{3\pi\sqrt{2}} \left( 1 - \frac{\omega_p-1}{p^2+2} \right) \int_0^\infty \frac{e^{-k^2/a^2}}{k^2+p^2+4} dk,$$

$$I_{21} = \frac{16\alpha\omega_p(\omega_p-1)}{3\pi\sqrt{2}(p^2+2)} \mathcal{P} \int_0^\infty \frac{e^{-k^2/a^2}}{k^2-p^2} dk.$$

The integrals involved in  $I_{20}$  and  $I_{21}$  will be:

$$\int_0^\infty \frac{e^{-k^2/a^2}}{k^2+p^2+4} dk = \frac{1}{a} \left[ 1 - \frac{2}{\sqrt{\pi}} \int_0^{\tilde{p}} e^{-t^2} dt \right] \frac{\pi}{2} \frac{e^{\tilde{p}^2}}{\tilde{p}},$$

$$\mathcal{P} \int_0^\infty \frac{e^{-k^2/a^2}}{k^2-p^2} dk = -\frac{\sqrt{\pi}}{a} \frac{e^{-\tilde{p}^2}}{\tilde{p}} \int_0^{\tilde{p}} e^{t^2} dt.$$

As a result,  $I_2$  has the form:

$$I_2 = \frac{2}{3} \frac{\alpha a \tilde{p}}{\sqrt{2}} e^{\tilde{p}^2} \left[ 1 - \frac{2}{\sqrt{\pi}} \int_0^{\tilde{p}} e^{-t^2} dt \right] - \frac{4\alpha a \tilde{p}}{3\sqrt{2}\pi} e^{-\tilde{p}^2} \int_0^{\tilde{p}} e^{t^2} dt.$$

Finally,  $\text{Re } D$  will be written as:

$$\text{Re } D = 1 + \frac{4\alpha a}{3\sqrt{2}\pi} \left( 1 - \tilde{p} e^{\tilde{p}^2} \int_{\tilde{p}}^\infty e^{-t^2} dt - \tilde{p} e^{-\tilde{p}^2} \int_0^{\tilde{p}} e^{t^2} dt \right).$$

This result reproduces the quantity given by formula (5.10). For the imaginary part  $\text{Im } D$  by Sokhotskys formula, we get:

$$\text{Im } D = \frac{1}{3\pi} \int_0^\infty f_k^2 k^4 \omega_k \delta(\omega_k^2 - \omega_p^2) dk = \frac{1}{6\pi} f_p^2 p^3.$$

As a result,  $|D(\omega_k^2)|$  is expressed as:

$$|D|^2 = (\text{Re } D)^2 + (\text{Im } D)^2 = \frac{2}{9} \alpha^2 a^2 \left[ e^{-2\tilde{p}^2} \tilde{p}^2 + \frac{8}{2\pi} \left( 1 - \tilde{p} \int_{\tilde{p}}^\infty e^{-t^2} dt - \tilde{p} e^{-\tilde{p}^2} \int_0^{\tilde{p}} e^{t^2} dt \right)^2 \right].$$

The first term in formula (5.7) is easily calculated to be:

$$\frac{1}{4\pi^2} \int_0^\infty \frac{k^4 f_k^2}{(1+Q)} dk = \frac{3}{16} a^2.$$

In calculating the second term in (5.7) we will separate out integral  $I_p$  in it:

$$I_p = \int_0^\infty e^{-k^2/a^2} \frac{k^2(\omega_k \omega_p + \omega_k(\omega_k + \omega_p) + 1)}{(\omega_k + \omega_p)^2} dk.$$

As  $a \rightarrow \infty$ , it is equal to:

$$I_p = a^3 \frac{\sqrt{\pi}}{4} \left( 1 - \tilde{p}^3 e^{\tilde{p}^2} \int_{\tilde{p}}^\infty e^{-t^2} dt (2 + 4\tilde{p}^2) + 2\tilde{p}^4 \right) = \frac{a^3 \sqrt{\pi}}{4} (1 - \Omega(\tilde{p})),$$

where:

$$\Omega(\tilde{p}) = 2\tilde{p} \left\{ (1 + 2\tilde{p}^2) \tilde{p} e^{\tilde{p}^2} \int_{\tilde{p}}^\infty e^{-t^2} dt - \tilde{p}^2 \right\},$$

which corresponds to the expression  $\Omega(y)$  in (5.12). As a result, the second term in formula (5.7) will be:

$$\frac{1}{12\pi^4} \frac{4\pi\alpha}{\sqrt{2}} \int_0^\infty I_p p^4 f_p^2 \frac{\omega_p}{(\omega_p^2 - 1) |D(\omega_p^2)|^2} dp.$$

As  $a \rightarrow \infty$ , this expression takes on the form:

$$\frac{\alpha^2 a^4}{3\pi \sqrt{\pi}} \int_0^\infty (1 - \Omega(\tilde{p})) \frac{e^{-\tilde{p}^2}}{|D(\omega_{\tilde{p}}^2)|^2} d\tilde{p} = \frac{3}{16} a^2 q,$$

where  $q = q(0)$  is given by expression (5.12). Hence, finally for  $\Delta E$  (5.7) we get:

$$\Delta E = \frac{3}{16} a^2 (1 + q),$$

which corresponds to the first term in the right-hand side of (5.11).

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